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SPECTROSCOPIC STUDIES OF THE ELECTRONIC STRUCTURE OF METAL-SEMICONDUCTOR AND VACUUM-SEMICONDUCTOR INTERFACES

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The electronic structure and properties of semiconductor interfaces including both vacuum-semiconductor and metal-semiconductor interfaces as well as relevant metal and semiconductor materials have been investigated under this contract. cont.

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The emphasis has been on elucidating the electronic properties of these materials and their interfaces, e.g., metal-semiconductor Schottky barriers, which are of far reaching importance in such semiconductor devices as MOSFETS, CCD devices, photovoltaic devices, etc. Extensive studies of the electronic structure of semiconductor surfaces and interfaces and related metal surfaces have been performed as a function of surface preparation (including laser annealing), doping, thickness of adsorbed overlayers, etc. The principal technique used has been photoelectron spectroscopy (XPS and UPS - with an emphasis on angle-resolved studies using synchrotron radiation and yield spectroscopy); other techniques include electron energy loss spectroscopy, low energy electron diffraction and theoretical band structure methods. Our research (34 completed papers) has included studies of well-characterized surfaces of Si, Ge, GaAs, GaSb, GaP, diamond, Au, W, Ta, Al, Pd, and Si interfaces; and Ni, Cu, Fe, Co, Zn, Ru, La, Th, V_3Si, UTe, and USb crystals. Major achievements of our research program includes world-leading contributions to (1) the electronic structure of cleaned and annealed Si(111) surfaces, (2) accurate experimental determinations of electron energy vs momentum band dispersions $E(\vec{k})$ of selected materials (such $E(\vec{k})$ dispersions are of central importance in solid state physics in understanding the electronic, physical and chemical properties of materials), and (3) the development and application of surface core level spectroscopy, a promising new photoemission technique.

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I. HIGHLIGHTS

Significant and extensive progress in understanding the electronic structure and properties of semiconductor surfaces and semiconductor interfaces as well as selected metallic and semiconducting materials has been accomplished under Air Force Office of Scientific Research Contract F49620-80-C-0025 (Dec.'79-Nov.'80). Techniques which have been used include photoelectron spectroscopy (with an emphasis on angle-resolved photoemission using synchrotron radiation), low energy electron diffraction (LEED), and Auger spectroscoy, as well as novel materials preparation methods such as laser annealing and molecular beam epitaxy. In summary, 34 research papers have been published under this contract (see Section III) on (a) the electronic structure of semiconductor surfaces and interfaces, (b) the bulk electronic structure of semiconductors, metals and metallic compounds, (c) surface core level spectroscopy, (d) many-electron effects and (e) other surface/interface studies.

Major achievements of this program for the past year include:

(1) Seven papers on the electronic structure of surfaces and interfaces of Si, diamond and Ge which represent a world-leading contribution to the surface electronic strucuture of Group IV semiconductors. A highlight is the first definitive study of a single-domain cleaved Si(111)-(2×1) surface.

(2) Eleven papers on the bulk electronic band structure of semiconductors, metals, and metallic compounds (including angle-resolved photoemission mapping of energy band dispersions $E(\vec{k})$). This program continues to be a world leader in the subject of energy band dispersion mapping $E(\vec{k})$, a subject of central and continuing interest in condensed matter science.

(3) Six papers on the new subject of surface core level spectroscopy have been completed; this work has established us as a world leader in this new sub-area of photoemission spectroscopy, which has only become possible with the use of synchrotron radiation. Important new work on surface phase transitions, e.g., surface reconstruction has been done.

(4) Six papers on the electronic properties of adsorbates on metals and on photostimulated ion desorption, which is a promising new tool.

As selected examples, three major highlights are described in this section: (1) electronic structure determination of Si surfaces -- Si(111)-(2×1), (7×7) and (1×1), (2) band structure determination of a prototype transition metal -- Ni -- and several related metals, and (3) the first surface core level spectroscopy study of a semiconductor -- GaAs.

Electronic Structure of the Si(111)-(2×1), -(7×7) and -(1×1) Surfaces. The cleaved Si(111)-(2×1) surface has been studied quite extensively using LEED (low energy electron diffraction), angle-resolved photoemission, etc. and is widely believed to have a buckled surface (2×1) geometry in which alternate rows of surface atoms are raised and lowered (e.g., see discussion and references in Ref.1). Experimentally, there have been difficulties in preparing single-domain cleavages with reproducible photoemission features,[2-5] e.g., peak positions can vary up to ~0.5 eV and the amount of band dispersion measured along $\bar{\Gamma}\bar{J}'$ (the short 2x1 Brillouin zone direction) has varied from 0.5 eV to <0.1 eV. Along $\bar{\Gamma}\bar{J}$, (the long zone direction) no band dispersion data have been reported. We have taken care to prepare single-domain Si(111)-(2x1) cleavage surfaces which are stable and reproducible, and have studied polarization-dependent surface state bands throughout the surface Brillouin zone by using an imaging two-dimensional photoelectron spectrometer. We have measured surface state dispersions $E(\vec{k}_\parallel)$ along the main symmetry lines $\bar{\Gamma}\bar{J}'$ and $\bar{\Gamma}\bar{J}$. Also, we have measured the polarization dependence of surface state emission, which yields symmetries. By exposing the (2x1) cleaved surface to activated H, the Si(111)-H(1x1) surface is formed, and differences in emission from these surfaces help distinguish bulk states from surface states. Our main result is that we find two distinguishable surface states near the top of the valence band which exist in different areas of the surface Brillouin zone and exhibit different sensitivities to hydrogen exposure. These states cannot be described in terms of calculated surface bands reported to date for buckled surface geometries.[7-9] Empirically, we locate the two surface states in two different band gaps of the projected bulk band structure. We conclude that either the geometry of Si(111)-(2x1) has not yet been determined unambiguously or that the surface states cannot be described by a band-like model which is the basis of present calculations.

The annealed (111) surfaces of Ge and Si are observed to reconstruct in different ways: a (1x1) LEED (low-energy-electron-diffraction) pattern is obtained from the laser-annealed Ge(111)-(1x1) and Si(111)-(1x1) surfaces, a (2x8)-type pattern from thermally-annealed Ge(111) and a (7x7) reconstruction from thermally-annealed Si(111). Despite these differences, similar types of geometries have been proposed for all thermally-annealed surfaces, e.g., buckling models,[10,11] island-type microdomains[12] or (2x2) building blocks centered around vacancies.[13] Each of these models has a characteristic short-range order, or local bonding and can accomodate different long-range order for different surfaces as seen in LEED observations. Photoelectron spectroscopy (PES) directly yields information about the local bonding but is less sensitive to the long range order than LEED. Therefore, we have used PES to determine the electronic surface states and surface core levels associated with different Ge(111) and Si(111) surfaces (laser-annealed and thermally-annealed) and have looked for common features. We have found for all four annealed Si(111)-(1x1) and -(7x7) and Ge(111)-(1x1) and (2x8) surfaces that surface state emission near the top of the valence band is dominated by two surface states which have distributions in $\vec{k}$-space characteristic of a 1x1 unit cell. A striking result is that these two upper and lower surface states each have the same characteristic angular distribution for all for surfaces. We observe a semiconducting surface for Ge(111)-(2x8), Ge(111)-(1x1) and Si(111)-(1x1) and a weakly metallic surface for Si(111)-(7x7). Also, there is a surface core level feature common to all four surfaces which corresponds to about 1/4 monolayer of surface atoms with a large shift of 0.6-0.8 eV towards lower binding energy. These are the first findings that suggest that there is a common local bonding geometry not only for laser-annealed and thermally-annealed Si(111) surfaces, but also for both annealed Si(111) and annealed Ge(111) surfaces, even though thermally-annealed Si(111)-(7x7) and Ge(111)-(2x8) surfaces have different long-range order.

Energy Band Structure E(k) of Ferromagnetic Ni and several related metals (Co, Cu, Zn). Recently, we have done pioneering work in determining accurate energy band dispersions E(k) for various transition and noble metals using angle-resolved photoemission with polarized synchrotron radiation and a simple three-step direct transition model of photoemission. Such one-electron band dispersions are of central interest for understanding various physical and chemical properties of materials, including studies of d-band electronic structure, chemisorption, many-body effects, and itinerant ferromagnetism. Of particular interest are E vs $\vec{k}$ dispersions along high symmetry lines in momentum space, since these are most easily related to theoretical calculations and thus to physical and chemical properties. An extensively used method for determining such $E(\vec{k})$ dispersions is $h\nu$-dependent angle-resolved photoemission normal to a low index plane surface.

As an example, Fig.3 summarizes E(k) dispersions in the low index (111) direction for several close-packed 3d metals. Co and Zn have the hexagonal close-packed structure (hcp) whereas Ni and Cu are face-centered cubic (fcc). Along the threefold axis, the energy bands of both lattices can be compared. The (0001) line $\Gamma\Delta A\Delta\Gamma$ for the hcp lattice corresponds to the (111) line $\Gamma\Lambda L$ for the fcc lattice.

From Co through Zn, we observe a free-electron-like (parabolic) s,p-band with Λ_1-symmetry Δ_1, Δ_2 for the hcp lattice) which hybridizes with a set of d-bands. The bottom of the s,p-band lies about 9 to 10 eV below E_F for Co through Zn. This value is lower by several eV than the value extrapolated for the bottom of the higher-lying parabolic conduction bands and as given by comparisons with values obtained for the inner potential in low-energy electron diffraction experiments. This downwards shift of the lowest s,p-band is attributed to hybridization with the d-bands. An s,p-band gap at the L-point supports the Λ_1 surface state we have also seen for Co through Zn.[14]

There are two Λ_3-type d-bands which join the points Γ_{12} and Γ_{25}' (fcc-notation). This can be seen most clearly for Cu. For Co and Ni, there are two sets of ferromagnetically-split d-bands (spin up and down). Ferromagnetic exchange splittings of 1-1.25 eV are directly seen for the Γ-points of Co, while a splitting of ~0.3 eV near L is seen for Ni. For Zn there is a substantial spin-orbit splitting of the lower d-band, as is observed for the 4d- and 5d-metals. The position and width of the d-bands are related to each other, i.e., the lower the d-bands lie relative to the s,p-band, the narrower they become. For Zn, the d-bands have become almost flat (0.17 eV dispersion between Γ_6^+ and Γ_5^- versus 0.60 eV for the analogous band in Cu), which indicates that these states are at the boundary between delocalized ("itinerant") and localized ("core-like") states.

Angle-resolved photoelectron spectroscopy techniques have been used to accurately determine energy band dispersions $E(\vec{k})$ along all three symmetry lines. A complete description of the ferromagnetic energy bands of Ni at the X-point has been obtained, which is the most important region in k-space for determining physical properties, i.e., Fermi surface properties. In Fig.4, our experimentally-determined energy bands for Ni near the X-point[15,17] are shown in detail for all bands near E_F. Not shown are lower lying bands at X, i.e., X_1 = -3.3 eV and X_3 = -2.8 eV. We believe that this experimental energy band determination is the most detailed and accurate such photoemission study reported to date. Certain energy bands are not observed in our ARPES experiments because of symmetry selection rules (shown as dashed lines in Fig.2). The empty $X_{5\downarrow}$ band critical point value ($X_{5\downarrow}$ = 0.23 eV) is based on de Haas van Alphen data and Zornberg's[16] interpolated values (for PS IV and PS VI potentials) which have been scaled by the ratio of experimental vs. calculated d-band width. This value for $X_{5\downarrow}$ is the same as we obtain using the measured $X_{5\uparrow} = -0.12$ eV point and assuming the same splitting as the measured $S_{3\downarrow}-S_{3\uparrow}$ splitting (the S_3 bands connect to the X_5 critical points). We observe that the ferromagnetic exchange splitting δE_{ex} for the d-like valence bands of Ni depends on the symmetry character of the wave functions. In particular, states derived from t_{2g} tight binding orbitals (e.g., Γ_{25}', X_5) exhibit a larger exchange splitting than e_g-derived orbitals (e.g., Γ_{12} , X_2). This agrees with theoretical estimates based on self-energy calculations. The d-band widths as observed in photoemission are smaller than those determined by ab initio *ground* state *calculations*. This effect increases from Co to Ni, and is small for Cu. We have correlated this apparent d-band narrowing to the position and strength of two-electron excitations which are seen as satellite structures to the valence band emission.[15]

In summary, a long-standing problem has been the itinerant (band-like) versus localized (atomic) nature of the ferromagnetic transition metals Fe, Co, and Ni. Various theoretical studies of ground state properties, and various experimental studies such as de Haas van Alphen data for Fermi surfaces and angle-resolved photoemission data such as our studies of energy band dispersions and exchange splittings have clearly shown that an itinerant band picture is basically valid. However, several interesting correlation effects have been observed for these materials -- notably Ni -- such as two-electron satellites, unexpectedly narrow d-bands, unexpectedly small band-dependent exchange splittings, etc. which involve self-energy effects that are not included in the usual one-electron band structure calculations for the ground state. These effects, which have been most clearly seen in our photoemission studies, are playing an important role in on-going theoretical efforts aimed at improving our understanding of the electron structure of solids.

Surface Core Level Spectroscopy. With the use of synchrotron radiation and novel instrumentation, i.e., our custom high-flux 3-m TGM monochromator and novel high-resolution 2D electron spectrometer,[6] we have been able to achieve sufficient energy resolution (≅0.15 eV) and surface sensitivity (fraction of an atomic layer) to measure the changes in electron binding energy of core levels of surface atoms (outermost 1 or 2 atomic layers) relative to the underlying bulk atoms. We have performed the first studies of such surface core level shifts for transition metals as a function of atomic number[18] and crystallographic face-dependence,[19] and have applied the technique to the study of surface phase transitions, i.e., surface reconstruction.[19,20] Also, we have performed the first surface core level studies of semiconductors[21,22] i.e., for GaAs and Si.

These surface binding-energy shifts, which measure the change in the electrostatic potential at the core, yield new information on charge redistribution in the surface layer which accompanies the large reconstruction and/or relaxation that invariably occurs for semiconductors. GaAs(110) is the prototype surface since its atomic structure is the best understood of any semiconductor; there is general agreement that surface As atoms move outwards and surface Ga atoms move inwards, with a ~25° bond-angle rotation[5,6] and a charge transfer from Ga to As surface atoms.[7]

Figure 5 shows several angle-integrated photoemisison spectra[21] for Ga(3d), As(3d), and Sb(4d) core levels in GaAs and GaSb; a smooth background has been substracted in plotting the spectra in Fig.5. Since the escape depth for photoelectrons depends strongly on kinetic energy, surface-to-bulk core-level emission intensity ratios can be varied by using different photon energies. For GaAs, two spectra (circles) for each core level are displayed in Fig.1: one with a photon energy ~10 eV above threshold, which shows mainly the bulk emission (large escape depth); the other at a photon energy ~40 eV above threshold, which shows significant surface core-level emission (small escape depth). At the lower photon energies, emission from the spin-orbit-split core-level pair ($d_{5/2}$,$d_{3/2}$) from the bulk is clearly observed; at the higher photon energies, an additional set of surface core levels separated by the same spin-orbit splitting which is shifted relative to the bulk levels is observed. The surface (S) and bulk (B) $d_{5/2}$ core-level spectral contributions for Ga, As and Sb are indicated in Fig.5. In Fig.5, each experimental spectra (circles) has been numerically fitted with four Lorentzians, two for the bulk and two for the surface, with the same $d_{5/2}$ - $d_{3/2}$ spin-orbit splittings, intensity branching ratios, and spectral widths. The solid lines (T) and dashed lines B and S give the total, bulk, and surface contributions to the spectra, respectively. The fit to the data is seen to be excellent. For GaAs(110), we find that the surface Ga 3d level is shifted to larger binding energy by Δ_B = +0.28 eV, while the As 3d level is shifted to smaller binding energy by ΔE_B = -0.37 eV relative to their bulk counterparts. These energy shifts of the outermost Ga and As core levels are consistent with the scant available theoretical data, and will provide additional information on charge transfer, etc. when accurate calculations become available. Such calculations have not been done because of the lack of experimental data.

We have also performed studies[22] of surface core level shifts for the cleaved Si(111)-(2×1) surface and annealed Si(111)-(7×7) and Si(001)-(2×1) surfaces which have yielded new surface geometry information. For Si(100)-(2×1), ~0.5 monolayer of surface atoms are found shifted to smaller binding energy (-0.5 eV) relative to the bulk; this rules out symmetric pairing models which would give a full monolayer of surface atoms with equal core level shift. Si(111)-(7×7) and Si(111)-(2×1) show different surface 2p core-level spectra (e.g., 1/6 layer shifted -0.7 eV versus 1/2 layer shifted -0.4 eV), suggesting different geometries. Si(111)-(1×1)H exhibits first-layer (+0.26 eV) and second-layer (+0.15 eV) shifts.

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Figure Captions

Fig.1 Angular distribution of photoelectrons for the dominant surface states at ~0.15 eV and 0.7 eV below E_F for cleaved Si(111)-(2×1) (see text).

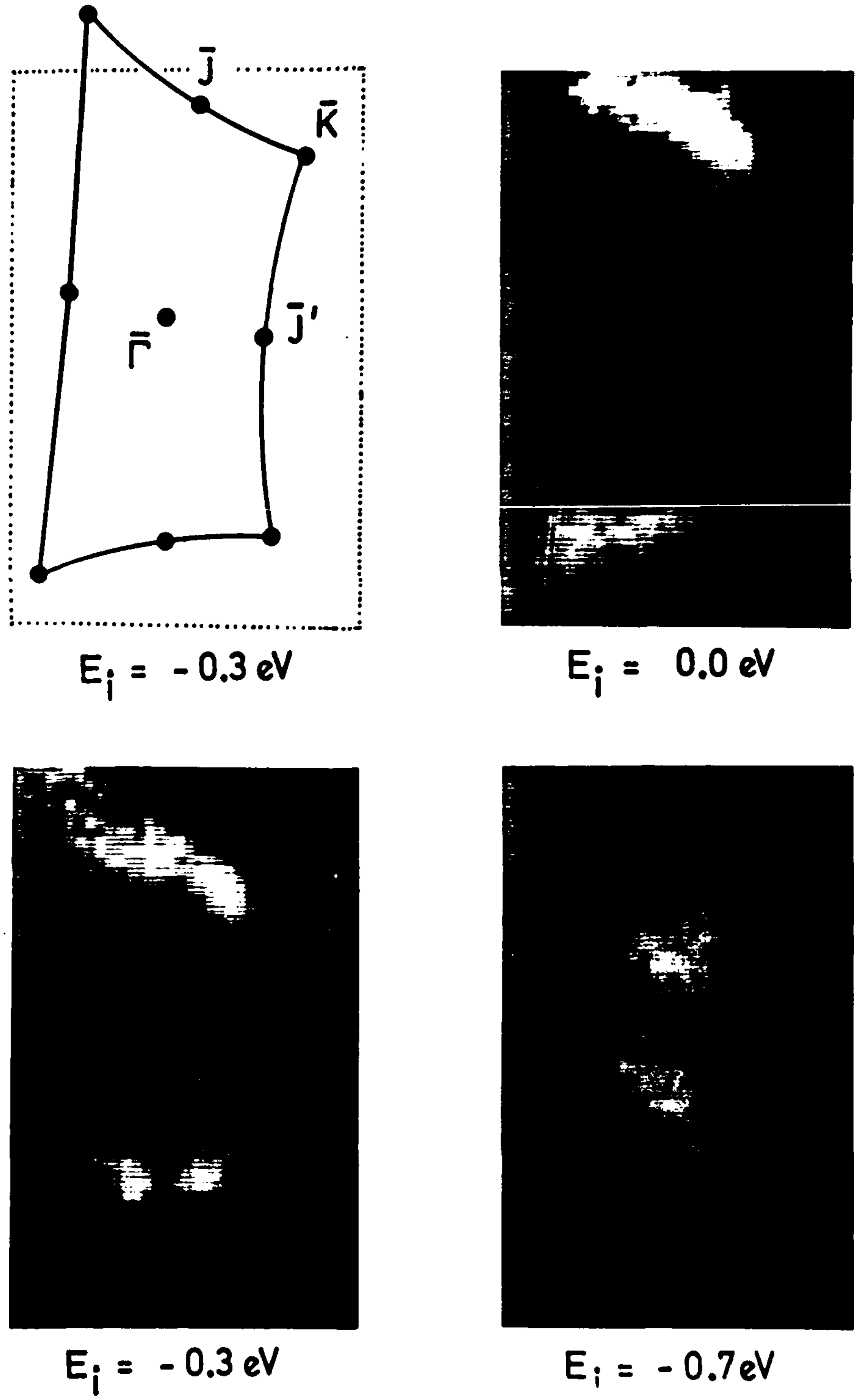
Fig.2 Angle-integrated photoelectron spectra for the annealed Ge(111) and Si(111) surfaces showing emission from two surface states near the top of the valence band which is quenched by hydrogen exposure (dotted lines).

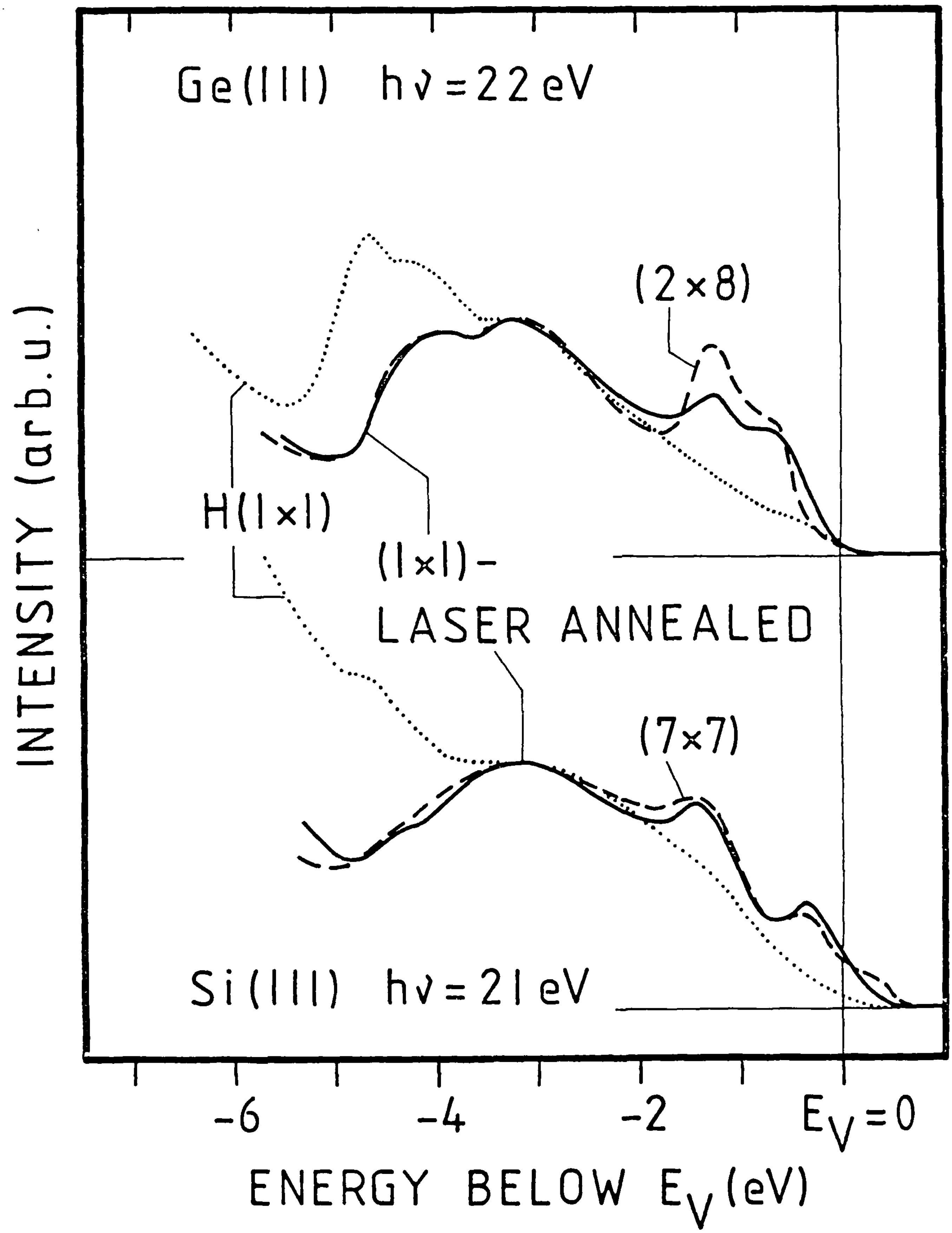
Fig.3 Experimental band dispersions along the threefold axis for Co, Ni, Cu and Zn. Circles are experimental data points. Majority spin bands are dashed for Co and Ni (From Ref.14).

Fig.4 Experimental energy bands of Ni (from Ref.15) near the X-point as seen in photoemission normal to a Ni(100) face (Δ-line) and normal to Ni(110) face (S-line). Triangles are de Haas van Alphen data.

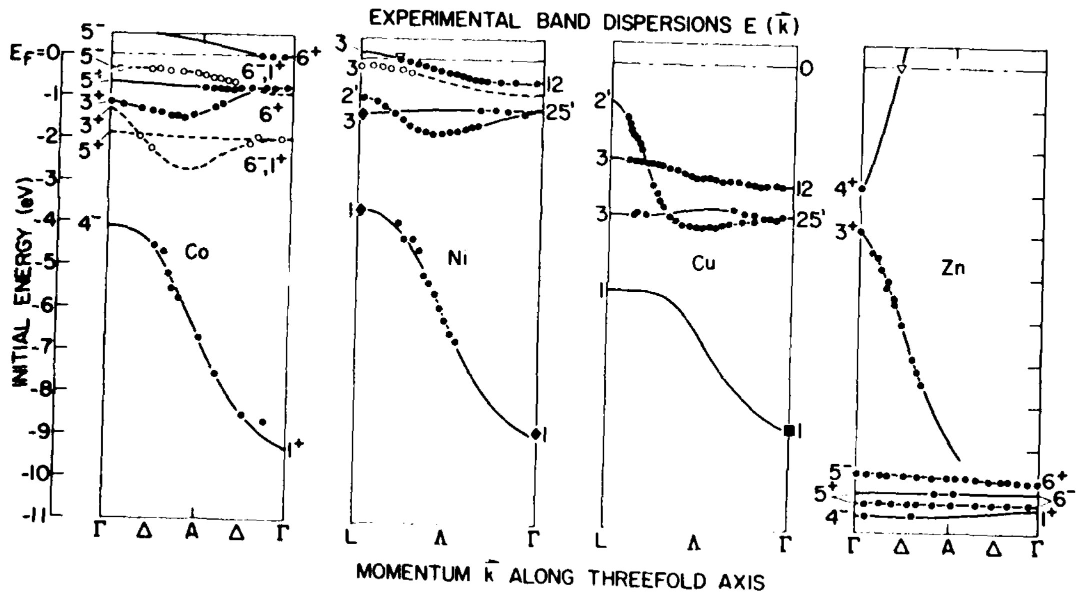
Fig.5 Photoelectron 3d and 4d core-level spectra with secondary-electron backgrounds (BG) subtracted (circles) and fitting results shown as solid and dashed curves for the total (T), bulk (B), and surface (S) contributions (after Ref.21).

Si(111)-(2x1) SURFACE STATES

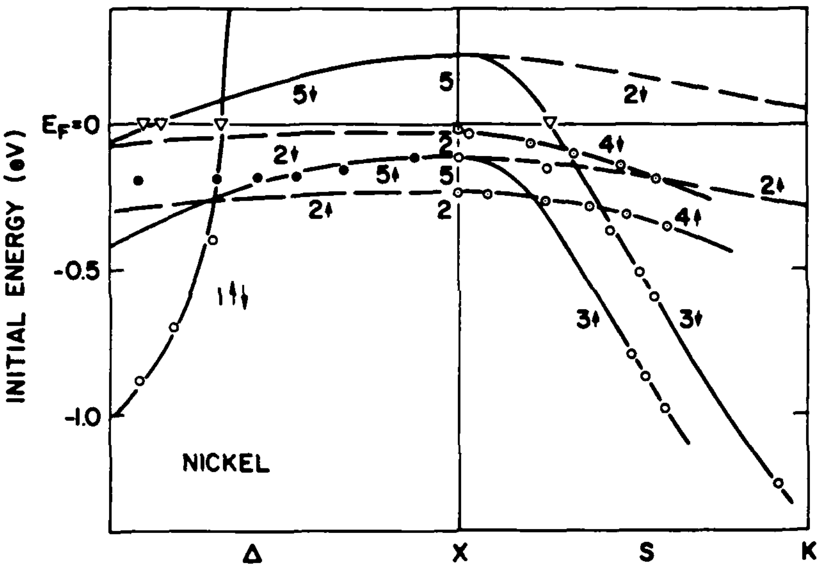




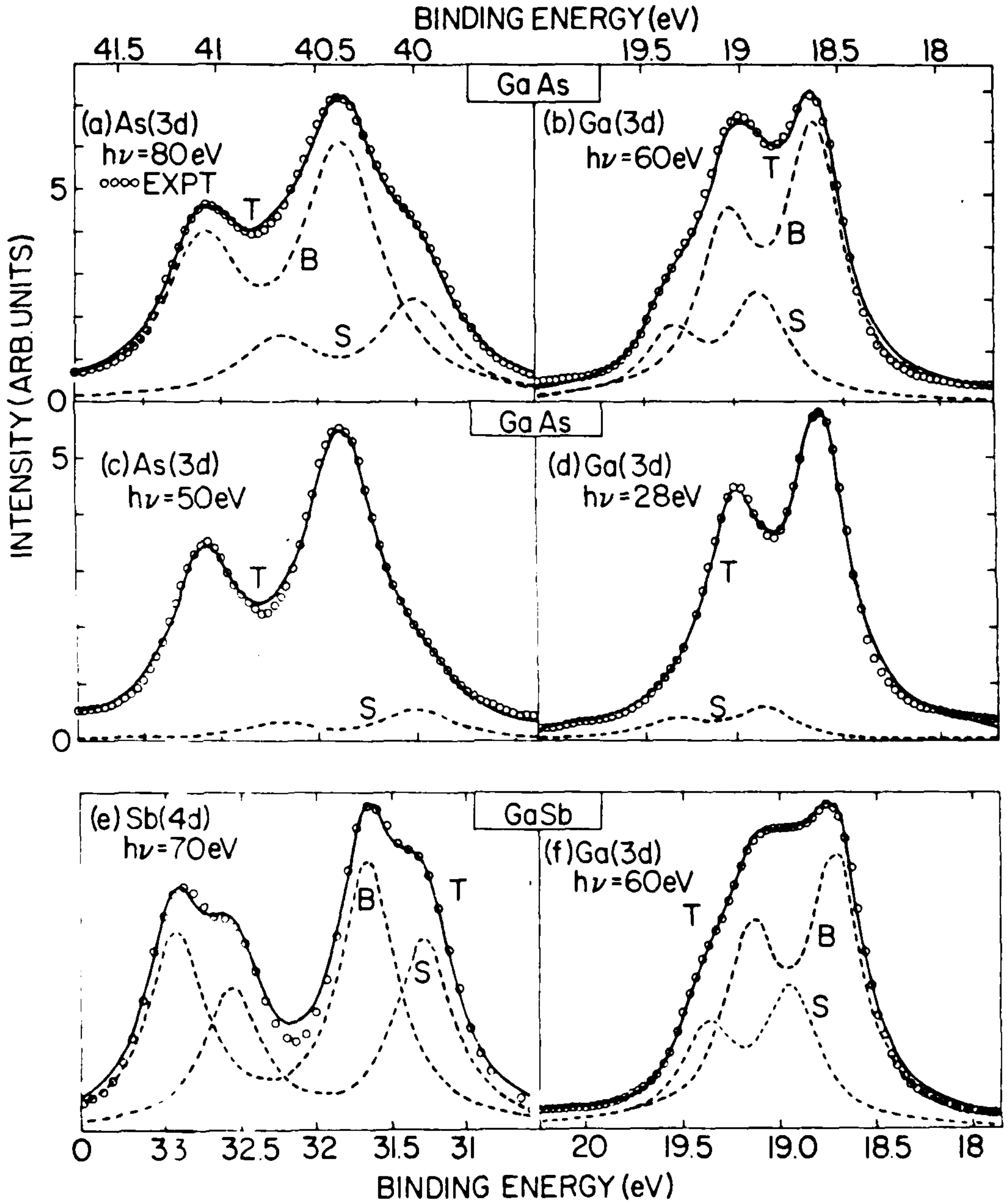
Ge(111) hν=22 eV
(2×8)
H(1×1)
(1×1)-
LASER ANNEALED
(7×7)
Si(111) hν=21 eV
INTENSITY (arb.u.)
-6
-4
-2
E_V=0
ENERGY BELOW E_V (eV)



EXPERIMENTAL BAND DISPERSIONS E ($\vec{k}$)
INITIAL ENERGY (eV)
E_F=0
Co
Ni
Cu
Zn
MOMENTUM $\vec{k}$ ALONG THREEFOLD AXIS



INITIAL ENERGY (eV)
$E_F=0$
-0.5
-1.0
NICKEL
Δ
X
S
K
5↓
5
2↑
2↓
2
4↓
5↓
5
2↓
2↑
2
4↑
1↑↓
3↑
3↓



BINDING ENERGY (eV)
41.5
41
40.5
40
19.5
19
18.5
18
GaAs
(a) As(3d)
hν=80eV
EXPT
T
B
S
(b) Ga(3d)
hν=60eV
T
B
S
INTENSITY (ARB. UNITS)
5
0
GaAs
(c) As(3d)
hν=50eV
T
S
(d) Ga(3d)
hν=28eV
T
S
5
0
GaSb
(e) Sb(4d)
hν=70eV
B
T
S
(f) Ga(3d)
hν=60eV
T
B
S
0
33
32.5
32
31.5
31
20
19.5
19.0
18.5
18
BINDING ENERGY (eV)

II. SUMMARY OF WORK COMPLETED UNDER CONTRACT

In the following, a brief summary of published research papers that were supported in part by the Air Force Office of Scientific Research under Contract F49620-80-C-0025 during the period December 1, 1979 to November 30, 1980. For clarity, these research papers (34 in all) have been grouped into five sub-areas of research:

A. Electronic structure of semiconductor surfaces and interfaces (Refs 1-7).
B. Bulk electronic structure of semiconductors, metals and metallic compounds (Refs
C. Surface core level spectroscopy (Refs 19-24).
D. Studies of many-electron effects (Refs 25-28).
E. Other surface/interface studies (Refs 29-34)

A. Electronic Structure of Semiconductor Surfaces and Interfaces

1. **Similarity Between the Si(111)-(7×7) and Impurity-Stabilized Si(111)-(1×1) Surfaces,**

Photoemission studies of intrinsic surface states are reported which show a strong similarity between the Si(111)-(7×7) and impurity-stabilized Si(111)-(1×1) surfaces. These results suggest that impurity-stabilized Si(111)-(1×1) surfaces are significantly reconstructed with a short range atomic configuration similar to that of the Si(111)-(7×7) surface, and are not unreconstructed with an essentially bulklike, contracted (1×1) surface as suggested via recent dynamical LEED calculations. (D.E. Eastman, F.J. Himpsel, and J.F. van der Veen, Sol. St. Commun., *35*, 345 (1980)).

2. **Schottky Barriers on Diamond(111)**

We have measured Schottky barrier heights $\phi_B = 1.3$ eV for Au and $\phi_B = 1.5$ eV for Al on (p-type) diamond(111)-(1×1) using photoelectron spectroscopy with synchrotron radiation. These barrier heights yield a barrier index of S = 0.2, which is closer to the values for Si and Ge (S ~0.1) than to the value S = 0.4 calculated for jellium on an ideal diamond(111) surface. After reacting Al with the diamond surface by annealing to 800°C, we find that ϕ_B decreases by 0.25 eV to 1.25 eV. (F.J. Himpsel, D.E. Eastman, and P. Heimann, Sol. State Commun. **36**, 631 (1980)).

3. **Electronic Surface Properties and Schottky Barriers for Diamond(111)**

Diamond is the prototype wide-gap semiconductor whose surface electronic properties are of interest in understanding group IV and group III-V semiconductor surfaces and interfaces. In previous LEED experimental surface studies, for diamond(111) a (1×1) surface and a reconstructed (2×2) surface have been observed via LEED. After heating the diamond(111)-(1×1) surface to about ~ 1000°C, we have obtained a 2×1/2×1 reconstructed surface. In contrast to the 1×1 surface, we find surface states near the top of the valence band and in the band gap for the 2×2/2×1 surface. Our as prepared diamond(111)-(1×1) surface exhibited no intrinsic surface states in the gap, and appears to be quite different from an ideal truncated bulk structure. (F.J. Himpsel, D.E. Eastman, J.F. van der Veen, J. Vac. Sci. Technol. *17*, 1085 (1980)).

4. **Surface States on Si(111)-(2×1)**

Surface state energy bands for a single-domain Si(111)-(2×1) surface have been studied with angle-resolved photoemission using synchrotron radiation. From the angular photoelectron distributions seen with a display-type spectrometer, we conclude that there are two surface states near the top of the valence bands E_v, one at E_v-0.7 eV around $\bar{\Gamma}$ (0.65 eV full width half maximum FWHM) and a second at E_v-0.15 eV(0.4 eV FWHM) along the line $\overline{JK}$. These states are found to be nearly dispersionless along the symmetry lines $\overline{\Gamma J'}$ and $\overline{JK}$. Their range of existence can be related to different gaps in the projected bulk bands. The lower surface state lies in a band gap above the L_3'-point which we find at E_v -1.5 eV. Our findings are not well-described by band calculations reported to date which use buckled-surface model geometries. Our results also indicate that several discrepancies among different reported experimental results are likely due to multi-domain cleavage effects. We conclude that either the geometry of Si(111)-(2×1) has not yet been determined unambiguously or that the surface states cannot be described by a band-like model which is the basis of present calculations. (F. J. Himpsel, P. Heimann, and D. E. Eastman, Phys. Rev. B (in press)).

5. **Similarity of the Laser- and Thermally-annealed Si(111) Surfaces**

Photoemission studies using synchrotron radiation show laser-annealed Si(111)-(1×1) and Si(111)-(7×7) surfaces have very similar electronic structures; namely, both show (i) the same two surface states (each with a characteristic angular emission pattern), (ii) similar surface core level spectra, and (iii) the same Fermi level pinning. We observe that the (1×1) and cleaved (2×1) surfaces are not related as recently reported. LEED studies conclude that the (1×1) surface has a compressed ideal (1×1) geometry; this is inconsistent with a band theory interpretation of our results. (D. Zehner, C.W. White, P. Heimann, B. Reihl, F.J. Himpsel, and D.E. Eastman, submitted to Phys. Rev. Lett.).

6. **A Study of Schottky Barrier Formation for Ga/Si(111)-(2x1) and Sb/Si(111)-(2x1) Interfaces**

We have studied the Schottky barrier formation of Ga/Si(111)-(2x1), Sb/Si(111)-(2x1) and Sb/GaAs(110) interfaces via photoemission measurements of the following coverage-dependent quantities: the Fermi level position at the interface relative to the valence band maximum E_V (i.e., p-type Schottky barrier Φ_B^P), work function, Si bulk and surface 2p core level binding energies, Ga 3d and Sb 4d core level energies, and Si surface states. Using a lightly-doped (~15 Ω-cm) p-type Si(111)-(2x1) sample which was cleaved with a single-domain (2x1) surface structure, we observe large deviations from the "1/3 band gap-rule" for p-type Schottky barriers Φ_B^P with both Ga and Sb; i.e., $\Phi_B^P \cong 0.07$ eV for Ga/Si(111) and $\Phi_B^P \cong 0.66$ eV for Sb/Si(111). The core level spectra for Ga and Sb for coverages in the 0.3 - 12Å range show very sharp core levels (observed FWHM ~ 0.4-0.5 eV), indicative of a "simple" interface without complex multiple binding sites or displacive reactions; this is in contrast with our studies of the Sb/GaAs(110) interface, for which the Sb core levels are significantly broadened (~ 1 eV FWHM) These studies are discussed in view of current models of Schottky barriers on covalent semiconductors. (J.L. Freeouf, M. Aono, F.J. Himpsel, and D.E. Eastman, J. of Vac. Sci. and Technol. (in press)).

7. **Electronic Structure of the Annealed Ge(111) and Si(111) Surfaces: Similarities in Local Bonding**

We have studied the valence band and surface-core-level states for thermally-annealed Ge(111)-(2×8) and Si(111)-(7×7) and laser-annealed Ge(111)-(1×1) and Si(111)-(1×1) surfaces with high resolution photoelectron spectroscopy using synchrotron radiation. We find two surface states near the top of the valence band which exhibit characteristic emission patterns within the hexagonal 1×1 surface Brillouin zone as well as characteristic surface core level spectra which indicate the existence of a common local bonding geometry for all these surfaces. (F.J. Himpsel, D.E. Eastman, P. Heimann, B. Reihl, C.W. White, D.M. Zehner, Phys. Rev. B (Rapid Commun.) in press).

B. Bulk Electronic Structure of Semiconductors, Metals, and Metallic Compounds

8. **Experimental Band Structure E(k) of V_3Si by Angle-Resolved Photoemission**

Band dispersions $E(\vec{k})$ and critical points of V_3Si have been determined by $\vec{k}$-selective angle-resolved photoemission with synchrotron radiation. A V-3d band ($\Delta_{1,2}$) which is very close to E_F at Γ (Γ_{12}) has been observed which is very flat near Γ along the ΓX direction, in agreement with recent APW calculations. Critical points of valence bands as well as their orbital character and density of states features have been determined. (M. Aono, F.J. Himpsel, and D.E. Eastman, submitted to Sol. State Commun.)

9. **Experimental Bulk Energy Bands for Diamond Using hν-Dependent Photoemission**

Using photon energy dependent photoemission techniques with a diamond (111)-(1×1) crystal surface, we have determined critical points of energy bands at Γ and L (Γ_1 = -21 eV, L_1 = -12.8 eV, L_2' = -15.2 eV, Γ_{15} = + 6.0 eV, Γ_2' = + 15.3 eV, L_2' = + 20 eV, Γ = + 24 eV with respect to the top of the valence band Γ_{25}'). Recent ab initio calculations agree with our results within 0.6 eV for the valence bands and show qualitative agreement for the empty conduction bands. The final bands are observed to be non-free-electron-like up to at least + 30 eV. (F.J. Himpsel, J.F. van der Veen, and D.E. Eastman, Phys. Rev. B*22*, 1967 (1980)).

10. **Experimental Energy Band Dispersions and Magnetic Exchange Splittings for Fe, Co, and Ni**

Using angle-resolved photoemission with single-crystal Fe(111) and Co(0001), we have determined accurate exchange-split energy-band dispersions $E(\vec{k})$ along symmetry lines. For Fe, Co, and Ni, respectively, occupied d-band widths are 3.1 eV (P), 3.8 eV (L), and 3.4 eV (L,X) while exchange splittings are ~ 1.5 eV (P), ~ 1.1 eV (Γ), and 0.3 eV (near L). Comparison with theory shows that state-of-the-art ab initio calculations describe the strong ferromagnets Fe and Co much better than Ni. (D.E. Eastman, F.J. Himpsel, and J.A. Knapp, J. of Mag. and Mag. Mater.,*15-18*, 1136 (1980)).

11. **Experimental E(k) Dispersions for the Zn 3d-states: Evidence for Itinerant Character**

Using angle-resolved photoemissson from Zn(0001) we observe that the Zn 3d states exhibit energy-band dispersions (0.17 eV from Γ_6^+ to Γ_5^- for the upper d band) and k-dependent polarization selection rules. The d bands are centered at 10 eV below the Fermi energy E_F and are 1.0 eV wide (Γ_4^- to Γ_5^-). In contrast, ab initio band calculations using a Hedin-Lundquist potential yield d bands centered at ~ 8.3 eV below E_F that are 1.5 eV wide and disperse by 0.33 eV, thus indicating the significance of self-energy corrections for these deep-lying narrow bands. Upon empirically correcting the d-band position by adjusting the exchange parameter α in a nonrelativistic $X\alpha$ calculation, the calculated bandwidth (1.0 eV) and dispersion are also in agreement with experiment. Experimental critical points are (energies relative to E_F): $\Gamma_5^- = -9.60eV, \Gamma_6^+ = -9.77eV$, $\Gamma_6^- = -10.05eV, -10.30eV$, $\Gamma_5^+ = -10.05eV, -10.31eV, \Gamma_4^- = -10.62eV$. The observed initial-state lifetime broadening (full width of half maximum) is 0.3 eV at the top of the d bands and 0.5 eV at the bottom of the d bands. (F.J. Himpsel, D.E. Eastman, E.E. Koch, and A.R. Williams, Phys. Rev. B**22**, 4604 (1980)).

12. **Experimental Energy Band Dispersions for Valence and Conduction Bands of Iridium**

Using angle-resolved photoemission with synchrotron radiation, we have determined the energy-versus-momentum dispersion relations $E(\vec{k})$ for the valence bands of Ir along the ΓΛL and ΓΔX symmetry directions. This has been achieved by measuring hν-dependent normal-emission spectra from Ir(111) and metastable unreconstructed Ir(100)-(1×1) surfaces. Conduction band critical points at Γ, X, and L are seen as structures in the angle-resolved energy spectrum of secondary electrons. Semi-empirical final bands were used to obtain E versus $\vec{k}$ energy dispersions of the initial bands. A strong resonance was observed for direct transitions at Γ from the upper d-bands (E = -1.04 eV relative to the Fermi level E_F) to an sp-like final-state band at E = +19.5 eV. The lower spin-orbit-split d-band and flat f-like final-state band (located at E ≅ +15 eV near Γ). Experimental energy bands are compared with Fermi surface data and a RAPW band structure calculation by Andersen. Surface "umklapp" scattering is shown to be important for bulk band emission from the (5×1) reconstructed Ir(100) surface. (J.F. van der Veen, F.J. Himpsel, and D.E. Eastman, Phys. Rev. B*22*, 4226 (1980)).

13. **Band Structure Measurements and Multi-electron Effects (Satellites) For Nearly-filled d-Band Metals: Fe, Co, Ni, Cu, Ru, and Pd**

Angle-resolved photoelectron spectroscopy has been used to determine energy band dispersions $E(\vec{k})$ along symmetry lines. A complete description of the ferromagnetic energy bands of Ni at the X-point has been obtained. We observe that the ferromagnetic exchange splitting δE_{ex} for the d-like valence bands of Fe, Co, and Ni depends on the symmetry character of the wave functions. In particular, states derived from t_{2g} tight binding orbitals (e.g., Γ_{25}', X_5) exhibit a larger exchange splitting than e_g-derived orbitals (e.g., Γ_{12}, X_2). This agrees with theoretical estimates based on self-energy calculations. The d-band widths as observed in photoemission are smaller than those determined by ab initio ground state calculations. This effect increases from Fe to Co to Ni, and is small for Cu, Ru and Pd. We correlate this apparent d-band narrowing to the position and strength of two-electron excitations which are seen as satellite structures to the valence band emission. (F.J. Himpsel, P. Heimann, and D.E. Eastman, 26th Conf. on Magnetism and Mag. Materials, November 1980, J. of Appl. Phys., in press).

14. **Experimental Energy Bands, Exchange Splittings, and Lifetimes for Ni in the Vicinity of the X-Point**

Angle-resolved photoelectron spectroscopy using synchrotron radiation has been used to determine energy band dispersions along the ΓKX and ΓX directions in nickel. A detailed picture of spin-dependent energy levels and band topology around the symmetry point X has been derived. We have measured the exchange splitting for different band symmetries and find the splitting for the X_2-S_4 band along (110) to be 0.17 eV. For the X_5-S_3 band we find a splitting of 0.33 eV which is in close agreement with the value found earlier for the Σ_2 band. This can be explained by different self-energy corrections for t_{2g} and e_g-type states respectively. Our values for the energy positions (inverse lifetimes) are the following: $X_{2\downarrow}$ = -0.04 eV (0.08 eV), $X_{2\uparrow}$ = -0.24 eV (0.19 eV), $X_{5\uparrow}$ = -0.11 eV. (P. Heimann, F.J. Himpsel, and D.E. Eastman, Sol. State Commun. (in press)).

15. **Experimental Energy Band Dispersions and Lifetimes for Ruthenium**

We have determined energy band dispersions and lifetimes for occupied and empty bands along the three-fold axis of Ru using angle-resolved photoelectron spectroscopy with synchrotron radiation. The lowest valence band extends from -7.5 eV below the Fermi level at Γ_1^+ to $-5.6 eV$ at Γ_4^- with an inverse lifetime of 1.2 eV. There is a band gap between -5.5 eV and -2.8 eV. The t_{2g}-like and e_g-like Γ-points are at -2.4 eV (Γ_6^-, Γ_1^+) and at -0.3 eV (Γ_6^+) respectively. A Δ_5, Δ_6-symmetry gap extends from -1.7 eV to -0.5 eV. A comparison with band calculations is given. (F.J. Himpsel, K. Christmann, P. Heimann, and D.E. Eastman, Phys. Rev. B *23*, 2548 (1981)).

16. **Free-Electron-Like Bulk and Surface States for Zn(0001)**

Energy versus momentum ($\vec{k}_{\parallel}$, k) energy band dispersions for s,p-like bulk and surface states of a Zn(0001) surface have been determined using angle-resolved photoemission with synchrotron radiation. We find nearly-free-electron (nfe) bulk s,p bands with an inner potential of $-15 < V_o < -13.5$ eV (below the vacuum level). At the zone boundary in the [0001] direction, the occupied s,p bands have a p-like critical point (Γ_3^+) at -3.9 eV below E_F and an s-like critical point (Γ_4^-) at -2.9 eV, while the nfe final states are found at +46 eV. These nfe final states appear to have slightly different energies (~2 eV) for transitions from occupied s- and p-states which can be described by an effective s- and p-dependent inner potential or by multiple band effects. A fully symmetric (Λ_1) s,p_z-like surface state is found at -3.6 eV in the $\Gamma_3^+\Gamma_4^-$ band gap; the band dispersion E vs. $\vec{k}_\parallel$ of this state has been measured over its full range of existence. The final state lifetime broadening ($2\Gamma \sim 4.5$ eV at +37 eV and $2\Gamma \sim 7$ eV at +54 eV final state energies, respectively) is reflected in large widths (~2-3 eV) of bulk s,p-band emission peaks. Surface state peaks are much narrower (0.7 eV) and are limited only by initial-state lifetime broadening. (F.J. Himpsel, D.E. Eastman, and E.E. Koch) Phys. Rev. B (in press).

17. **Evidence for Quasi-localized 5f Electronic States in USb_xTe_{1-x}**

We have studied the '5f,6d' electron states of the system USb_xTe_{1-x}(100) using photoemission spectroscopy with synchrotron radiation. In contrast with the generally accepted picture of U chalcogenides and pnictides, we find for UTe that the main 5f level lies 0.75 eV below E_F *rather* than at E_F and that 6d *states* exist at E_F. Our results may be explained with a model having a correlated quasi-localized $5f^{3-\delta}$ (δ=0-0.5) level resonant with broader 6d bands rather than band-like 5f levels. (B. Reihl, N. Martensson, P. Heimann, D.E. Eastman, and O. Vogt Phys. Rev. Lett. (in press)).

18. **Electronic Structure and Magnetism of $U_xTh_{1-x}Sb$ as Studied by Photoemission**

Using photoelectron spectroscopy with synchrotron radiation in the $10 \leq h\nu \leq 130$ eV range, we have studied the '5f,6d' electron states in single crystal $U_xTh_{1-x}Sb$. We find that uranium has a quasi-localized 5f resonant level with essentially a trivalent configuration and does not change valence in the ordered magnetic region $1.0 \geq x \geq 0.3$, while thorium contributes 6d conduction band electrons which play an important role in both the electronic and magnetic properties. (B. Reihl, N. Martensson, D.E. Eastman, and O. Vogt, Phys. Rev. B (in press)).

C. Surface Core Level Spectroscopy

19. **Surface Core Level Binding Energy Shifts for GaAs(110) and GaSb(110)**

Surface 3d and 4d core-level binding-energy shifts have been resolved in photoemission from GaAs(110) and GaSb(110), which yield new information on semiconductor-surface reconstruction. The shifts (~0.3 eV) are toward higher (lower) binding energies for the surface cations (anions), in agreement with a simple model involving the known surface relaxation of GaAs(110) with a geometry-dependent initial-state charge transfer. Surface core-excitation binding energies, core-level widths, escape depths, etc., are reevaluated. (D.E. Eastman, T.-C. Chiang, P. Heimann, and F.J. Himpsel, Phys. Rev. Lett. *45*, 656 (1980)).

20. **Geometry-dependent Si(2p) Surface Core Level Excitations for Si(111) and Si(100) Surfaces**

We report structure-dependent Si(2p) surface core level shifts and 2p photothreshold spectra which yield new surface geometry information. For Si(100)-(2×1), we find ~0.5 monolayers of surface atoms shifted to smaller binding energy (-0.5 eV) relative to the bulk; this rules out symmetric pairing models. Si(111)-(7×7) and Si(111)-(2×1) show different surface 2p core level spectra (e.g., 1/6 layer shifted -0.7 eV vs 1/2 layer shifted -0.4 eV), suggesting different geometries. Si(111)-H(1×1) exhibits first layer (+0.26 eV) and second layer (+0.15 eV) shifts. (F.J. Himpsel, P. Heimann, T.-C. Chiang, and D.E. Eastman, Phys. Rev. Lett., *45*, 1112 (1980)).

21. **Structure-dependent Surface Core Level Shifts for the Au(111), (100), and (110) Surfaces**

We have measured 4f core-level shifts and surface-to-bulk intensity ratios for surface atoms on the Au(111), (100) and (110) faces. These shifts show crystallographic dependences as well as dependences on surface reconstruction. For the reconstructed Au(110)-(2x1) surface, our data are consistent with a relaxed missing row model and exclude an unrelaxed missing row model. The Au(100)-(5x20) reconstructed surface gives surface core-level shifts and intensity ratios which are consistent with a buckled hexagonal overlayer model with surface relaxation. (P. Heimann, J.F. van der Veen and D.E. Eastman Sol. State Commun. (in press)).

22. **Observation of Opposite 4f-Surface Core Level Binding Energy Shifts for W(111) and Ta(111)**

Surface 4f core level binding energy shifts have been measured in photoemission from W(111) and Ta(111). The surface shift was found to change sign across the row of 5d-metals: for the topmost layer of Ta(111) a +0.40 eV shift toward higher binding energy is found, whereas for W(111) the shift is -0.43 eV toward lower binding energy. The shifts are shown to be dependent on surface crystallography. Chemical shifts are determined for saturation coverage of hydrogen. (J.F. van der Veen, P. Heimann, F.J. Himpsel, and D.E. Eastman, Sol. State Commun. *37*, 555 (1981).

23. **Core Level Shift at a Jellium-Like Surface: Al(001)**

The shift of 2p core level binding energies associated with surface atoms relative to bulk atoms for an Al(001) surface has been determined using photoemission partial yield techniques. The observed shift is -57 meV. A possible mechanism for the core level shift is discussed using a simple jellium model, i.e., the shift is related to the Friedel oscillations in the electrostatic potential associated with the conduction electron response to the jellium-like surface potential step. (T.-C. Chiang and D.E. Eastman, submitted to Phys. Rev. B (Rapid Commun.)).

24. **Surface Core-Level Shifts and Surface Valence Change in Mixed-Valent $YbAl_2$**

High-resolution photoemission studies show that about two surface layers of mixed-valent $YbAl_2$ are divalent and dominate the spectra from $30 \leq h\nu \leq 110$ eV. These layers exhibit large surface core-level shifts of up to $\cong 1$ eV. A mean valence of 2.4 ± 0.1 is found for bulk $YbAl_2$, and its change at the surface is explained via a thermochemical analysis of the surface core-level shifts. A recently proposed core-hole induced valence change mechanism for related mixed-valent $YbAl_3$ is strongly questioned. (G. Kaindl, B. Reihl, D.E. Eastman, R. Pollak, N. Martensson, B. Barbara, T. Penney, and T. Plaskett, submitted to Phys. Rev. Lett.).

D. Studies of Many-electron Effects

25. Multielectron Effects in Photoemission from Quasi-Atomic Copper in Cu-Phthalocyanine

Photoelectron energy distribution curves for Cu in Cu-Phthalocyanine have been investigated in the photon energy range from $h\nu = 20$ eV to 130 eV. At the Cu 3p threshold at $h\nu = 75$ eV a sharp 3d-electron satellite with two peaks with initial energies of 5.5 eV and 8.5 eV below the center of the Cu 3d main peak was found which exhibits a strong resonant enhancement while the cross section for the Cu 3d-derived maximum shows a sharp minimum at threshold. These results are explained as a two-electron shake-up multiplet with a $3p^6\, 3d^8\, 4s^2 + e^-$ final state configuration. The results are compared to metallic Cu, and the different chemical, relaxation (screening) and configuration shifts are discussed. (M. Iwan, E.E. Koch, T.-C. Chiang, D.E. Eastman, and F.J. Himpsel, Sol. State Comm. ***34***, 57 (1980)).

26. Observation of the Transition from Uncollapsed to Collapsed Excited f-Wave Functions in I^-, Xe, and Cs^+ via Giant PCI Auger Effect

The nature of the final f-wave functions, i.e., spatially collapsed vs uncollapsed, involved in $4d \rightarrow 4\epsilon f$ giant absorption resonances in I^-, Xe, and Cs^+ is revealed by studying the post-collision-interaction (PCI) in the $N_{4,5}O_{2,3}O_{2,3}$ Auger decay of the 4d hole. While small PCI Auger shifts $\lesssim 0.2$ eV are observed for I^- and Xe with uncollapsed f-wave functions, a giant PCI Auger shift of ~1 eV is observed for Cs^+ with collapsed f-wave functions. (T.-C. Chiang, D.E. Eastman, F.J. Himpsel, G. Kaindl, and M. Aono, Phys. Rev. Lett. **45**, 1846 (1980)).

27. Delayed Onset of 4d Photoemission Relative to the Giant 4d Photoabsorption of La

For the giant 4d photoabsorption of La, both the total photoabsorption spectrum and the $N_{4,5}$-derived Auger emission intensity spectrum increase significantly above $h\nu \cong 112$ eV, with spectral peaks at $h\nu = 118$ and 119 eV, respectively. However, the predominant 4d photoemission partial cross section shows a delayed onset of ~ 4 eV, with a peak at $h\nu = 121$ eV, while the 5s, 5p, and 5d partial cross sections all show a strong resonant enhancement at lower energies, with spectral peaks at $h\nu = 116.6$ eV. These results are compared with a recent many-body calculation for Ce. The photon energy dependence of the La $4d_{5/2}/4d_{3/2}$ photo-emission branching ratio is consistent with a "final-state model." (M. Aono, T.-C. Chiang, F.J. Himpsel, and D.E. Eastman, Sol. State Commun. *37*, 471 (1981).

28. **Anomalous Two-Electron Auger Resonance in Thorium Near the 5d(O_5) *Photothreshold***

The photoexcited O_5P_3V Auger emission line for thorium metal shows an anomalous increase in kinetic energy of ~1 eV as the photon energy $h\nu$ is increased through the atomic-like $5d \rightarrow 5f$ resonant excitation at $h\nu_r = 89$ eV. Possible mechanisms for this anomalous behavior are discussed, and it is suggested that it can be interpreted as a two-electron resonance involving the O_5P_3V Auger excitation and a shake-up satellite of the $6p_{3/2}$ core level excitation. (M. Aono, F.J. Himpsel, T.-C. Chiang, J.H. Weaver, and D.E. Eastman, submitted to Sol. State Commun.).

E. Other Surface/Interface Studies

29. **Distance-Dependent Relaxation Shifts of Photoemission and Auger Energies for Xe on Pd(001)**

Photo- and Auger-electrons from Xe in adsorbed multilayers of Xe on Pd(001) as well as on spacer layers of Kr on Pd(001) exhibit well-resolved increases in kinetic energy with decreasing distance from the surface (28-2 Å), allowing a direct labelling of the layers. These relaxation shifts for core-hole excitations (0.9 - 2.1 eV) and for Auger excitations (3.3 - 6.6 eV) are well described by an image potential, where the position of the image plane agrees within 0.2 Å with local-density functional theory. (G. Kaindl, T.-C. Chiang, D.E. Eastman, and F.J. Himpsel, Phys. Rev. Lett. *45*, 1808 (1980)).

30. **Angular Dependent Photon-Stimulated Desorption of Ions from a $V_2O_5(010)$ Surface**

Using a display-type analyzer, we have measured the angular and energy distribution of O^+ ions desorbed from a $V_2O_5(010)$ surface by incident photons. The desorbed ions were mass-analyzed using time-of-flight gating techniques. The angular distribution of desorbed ions was found to be strongly peaked in the direction of the surface normal. This strongly directional desorption pattern reflects the local bonding geometry of the topmost oxygen atoms in the surface. The observed photoexcitation spectrum of the ion yield can be explained with the core level Auger decay model formulated by Knotek and Feibelman. (J.F. van der Veen, F.J. Himpsel, D.E. Eastman, P. Heimann, Sol. St. Commun. *36*, 99 (1980)).

31. **Layer-Dependent Core-Level Shifts for Rare-Gas Adsorbates on Metals**

Photo- and Auger-electrons from rare-gas atoms (Xe, Kr) physisorbed in form of monolayers, bilayers, and multilayers on metal surfaces (Pd(001)) exhibit well-resolved increases in kinetic energy with decreasing distance from the surface. The observed shifts are well described as extra-atomic hole-relaxation effects, using a point-charge image-potential model. They allow a direct labeling of the first few layers of an adsorbed multilayer configuration and are used to study the thermally-activated inversion of Kr/Xe bilayer on Pd(001). (G. Kaindl, T.-C. Chiang, D.E. Eastman, and F.J. Himpsel, Ordering in Two Dimensions, S.K. Sinha, editor, North Holland, 1980 (in press)).

32. **Photoemission from Physisorbed CO on Clean and Xe-covered Al(111)**

Molecular-orbital energy shifts are observed in photoemission from weakly physisorbed CO on clean and Xe-covered Al(111) surfaces. These shifts in ionization potentials are mainly due to final-state relaxation effects, which can be described approximately by a point-charge image-potential model. Differential distance- and orbital-dependent energy shifts suggest that CO molecules lie flat on the substrates. CO is adsorbed on Al(111) with a heat of formation of 0.21 eV/molecule. (T.-C. Chiang, G. Kaindl, and D.E. Eastman Sol. St. Commun. **36**, 25 (1980)).

33. **Photoemission Studies of Ar, Kr, and Xe Adsorbed on Al(111)**

S ıbmonolayers of rare gases adsorbed on Al(111) have been studied using photoemission techniques. Coverage-dependent core level binding energy shifts and work-function changes have been measured; polarizabilities and dipole moments are deduced. Results indicate that adatom spatial distributions for Xe submonolayers adsorbed on Al(111) at 40K are best described by a random 2-dimensional distribution, and there is negligible charge transfer from the Al substrate onto the Xe adatoms in the photoionization process. (T.-C Chiang, G. Kaindl, and D.E. Eastman submitted to Phys. Rev. Lett. (Feb. 1981)).

34. **Inversion Kinetics for Kr/Xe Bilayers on Palladium**

The thermally-activated inversion of Kr/Xe bilayers on Pd is studied using photoemission and photon-excited Auger spectroscopy. Bilayers formed by depositing a monolayer or less of Xe on top of a monolayer of Kr on Pd at 49K are shown to invert when the temperature is raised, with Xe coming in direct contact with the substrate. For a Pd(111) substrate, the activation energy of the inversion process is determined: $E_a = 0.12 \pm 0.03$ eV. (G. Kaindl, T.-C. Chiang, and D.E. Eastman, submitted to Phys. Rev. Lett.).

III. LIST OF PUBLICATIONS UNDER CONTRACT

A. Electronic Structure of Semiconductor Surfaces and Interfaces.

1. D.E. Eastman, F.J. Himpsel, and J.F. van der Veen, Similarity Between the Si(111)-(7×7) and Impurity-Stabilized Si(111)-(1×1) Surfaces, Sol. St. Commun., *35*, 345 (1980).

2. F.J. Himpsel, D.E. Eastman, and P. Heimann, Schottky Barriers on Diamond(111), Sol. State Commun. **36**, 631 (1980).

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IV. Biography of Principal Investigator

Dean E. Eastman received his B.S., M.S., and Ph.D. in Electrical Engineering from the Massachusetts Institute of Technology in 1962, 1963, and 1965, respectively. He joined the IBM Research Division as a Research Staff Member in 1963, where he has been since 1965 except for a year (1972-1973) as a Visiting Professor at M.I.T. He began his position as an IBM Fellow in 1974, and has held research management positions since 1971. Currently, he is manager of the Surface Physics and Photoemission Group, with research activities at the IBM Research Center and at the Synchrotron Radiation Center at the University of Wisconsin - Madison.

Eastman's research has been in condensed matter physics. His principal contributions have involved the development of new photoemission spectroscopy techniques and their applications to a broad range of studies of the electronic structure of solids and surfaces, including intrinsic surfaces, chemisorption and semiconductor interfaces. Selected examples include the development of accurate experimental one-electron band dispersions $E(\vec{k})$ techniques using angle-resolved photoemission and their application to metals, semiconductors and metallic compounds; surface science contributions include the application of UV photoemission to the study of the electronic states of chemisorbed atoms and molecules, studies of relaxation effects, and measurements of one-electron band dispersion $E(\vec{k})$ for intrinsic electronic surface states on metals and semiconductors. He has contributed substantially to the advancement of photoemission techniques -- including the development of UHV differentially-pumped He/Ne resonance radiation sources, the use of synchrotron radiation, and the development of a 2D area detector for energy- and momentum-resolved studies. He has published about 170 papers in the areas of photoelectron spectroscopy, ultrasonics, microwave resonance, and x-ray lithography.

Credits

IBM Fellow

Fellow, American Physical Society

Chairman, Solid State Sciences Committee of the National Academy of Sciences, 1979-present.

Oliver E. Buckley Solid State Physics Prize, 1980.

At various past and present times:

- Councillor-at-Large of the American Physical Society
- National Science Foundation Advisory Committee for Condensed Matter Sciences,
- Solid State Sciences Panel of the National Academy of Sciences,
- APS Davisson Germer Prize Committee,
- APS Buckley Prize Committee; Chairman
- Users Executive Committee of the Synchrotron Radiation Center at the University of Wisconsin-Madison,
- Proposal Review Committee of the Stanford Synchrotron Radiation Laboratory,
- Advisory Committee for the National Synchrotron Light Source at Brookhaven National Laboratory,
- Associate Editor of the Journal of Electron Spectroscopy,
- Co-Editor of the Handbook on Synchrotron Radiation,
- Served on several NAS/NRC Study Panels as well as on numerous program committees for national and international conferences.

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